

1H-Imidazole-2-sulfonic acid  
53744-47-1 | DTXSID40601515

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $1.34 \times 10^{-11}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Outside

**Local applicability domain index:**  $2.39 \times 10^{-1}$

**Confidence level:**  $6.13 \times 10^{-1}$

## Nearest Neighbors from the Training Set

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2,5-Furandione

**Measured:**  $1.45 \times 10^{-12}$

**Predicted:**  $2.17 \times 10^{-12}$

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2(3H)-Furanone

**Measured:**  $4.45 \times 10^{-11}$

**Predicted:**  $3.74 \times 10^{-11}$

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Glyoxal

**Measured:**  $1.14 \times 10^{-11}$

**Predicted:**  $1.14 \times 10^{-11}$